On the behavior of a 2D Heisenberg antiferromagnet at very low temperatures

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We present an analytical result for the ratio of the physical correlation length in a 2D Heisenberg antiferromagnet on a square lattice, and the one which is actually computed in numerical simulations. This last correlation length is deduced from the second moment of the structure factor at the antiferromagnetic momentum Q. We show that the ratio is very close to one in agreement with previously obtained numerical result of the $1/N$ expansion.

The two-dimensional Heisenberg antiferromagnet on a square lattice is one of the most extensively studied systems in condensed-matter physics. The interest to this model is two-fold. On one hand, Heisenberg antiferromagnet models a large number of real materials including parent compounds of high-T_c superconductors. On the other hand, its low-energy physics is adequately described by a field-theoretical $\sigma-$model thus allowing one to find similarities between condensed-matter physics and field theory.

The low-temperature behavior of the Heisenberg antiferromagnet is understood in great detail. For short-range interaction, the ground state is ordered unless one fine tunes the couplings between nearest and further neighbors. The ordered ground state is characterized by a sublattice order parameter, N_0, spin stiffness, ρ_s, and transverse susceptibility, $\chi_\perp = c^{-2}\rho_s$, where c is the spin-wave velocity. At any finite temperature, however, the system is disordered due to thermal fluctuations. The disordering means that equal-time spin-spin correlation function decays exponentially with the distance, as $e^{-r/\xi}$. The length scale ξ is the physical spin correlation length. Various approaches to $2D$ antiferromagnets all predict that in the renormalized-classical region ($T \ll \rho_s$) which we only consider here, ξ is exponentially large in T at low T and behaves as $\xi \sim \frac{c}{2\pi\rho_s} \exp(\frac{2\pi\rho_s}{T})$. Equal-time spin correlations at large distances can also be described by a static structure factor $S(k)$ for k near the antiferromagnetic momentum $Q = (\pi,\pi)$. In the disordered spin state, $S(Q)$ scales as ξ^2 and is therefore also exponential in T.

The exponential temperature dependences of ξ and of $S(Q)$ have been verified in numerical simulations and by analyzing the neutron scattering and NMR data for La_2CuO_4 and $Sr_2CuO_2Cl_2$. The accuracy of numerical simulations is so high, however, that one can not only check the temperature dependences but also compare the absolute values of the structure factor and the spin correlation length. There is, however, one subtlety in the numerical analyses - in numerical simulations, one measures not the physical spin correlation length, but another length scale which is also exponentially small

in T, but generally differs from ξ by a constant factor. Indeed, the physical spin correlation length can be extracted from the form of $S(k)$ simply because Fourier-transform of $S(k)$ yields the spin correlation function in real space. However, one can easily make sure that the long-distance behavior of $S(r)$ is associated with the form of $S(k)$ along the *imaginary* k-axis. Moreover, the inverse spin correlation length is the scale at which $S(k)$ has a pole for imaginary k: $S^{-1}(k = i\xi^{-1}) = 0$. In numerical simulations, however, the structure factor is evaluated only for *real* values of momentum k. Accordingly, a different definition of the correlation length is employed - it is identified as a second moment of $S(k)$ for $k = Q$, i.e., as $\tilde{\xi} = (-S^{-1}(Q)dS(k)/dk^2|_{k \to Q})^{1/2}$. For the Lorentzian form of $S(k)$, $S(k) \propto ((Q - k)^2 + m_0^2)^{-1}$, both ξ and $\tilde{\xi}$ are equal to the mean-field spin excitation gap m_0 and are therefore undistinguishable. However, the $1/N$ calculations for the $O(N)$ $\sigma-$model rigorously demonstrated that $S(k)$ has a Lorentzian form only in the limit $N \to \infty$ while for arbitrary N, and, in particular, for physical $N = 3$, $S(k)$ possesses a much more complex dependence on k which arizes due to temperature-independent $1/N$ corrections. In this situation, $\tilde{\xi}$ and the physical spin correlation length ξ differ by some constant factor. This factor appears to be a relevant one as several groups [1,2] recently performed a detailed comparison of $\tilde{\xi}$, calculated numerically at very low T, with the exact expression for ξ obtained some time ago by Hasenfratz and Niedermayer (see below). In this analysis, they assumed that ξ and $\tilde{\xi}$ are almost the same. *A priori*, however, there are no reasons for such coincidence.

We start by quoting the seminal result [3] that

$$\xi^{-1}/m = \left(\frac{8}{e}\right)^{1/(N-2)} \frac{1}{\Gamma(1 + 1/(N-2))}, \qquad (1)$$

where m is given by

$$m = \frac{T}{c} \left(\frac{2\pi\rho_s}{(N-2)T}\right)^{\frac{1}{N-2}} e^{-\frac{2\pi\rho_s}{(N-2)T}}. \qquad (2)$$

This result is based on numerical results for $N = 3$ and $N = 4$ [3] and on $1/N$ expansion for $O(N)$ $\sigma-$model [4,5].

For $N = 3$, this yields $\xi^{-1}/m = (8/e) \approx 2.94$. No such exact expression, however, exists for $\tilde{\xi}$. The $1/N$ expansion for $O(N)$ σ model (which in the renormalized-classical region holds in powers of $1/(N - 2)$ [7]) yields

$$\tilde{\xi}^{-1} = \xi^{-1}(1 + 0.003/(N - 2)), \qquad (3)$$

where factor 0.003 arises from numerical evaluation of some complicated integrals. A formal application of this result to a physical case of $N = 3$ yields almost identical values for $\tilde{\xi}$ and ξ. It is known, however, that a special care has to be taken in this procedure as not all terms which appear to first order in $1/(N - 2)$ actually contribute at $N = 3$. To illustrate this point, consider large N expansion for ξ^{-1}/m. An analytical evaluation of the first $1/N$ correction yields

$$\xi^{-1}/m = \left(1 + \frac{1}{N - 2}\left(\log(8/e) + \gamma_E\right)\right) \qquad (4)$$

where γ_E is the Euler constant. Comparing this formula with the exact result, Eq. (1), we notice that the Euler constant accounts for the appearance of the Γ function in (1): $\Gamma(1 + 1/(N - 2)) = 1 - \gamma_E/(N - 2) + O(1/(N - 2)^2)$. As $\Gamma(2) = \Gamma(1) = 1$, the term with the Euler constant does not contribute to ξ^{-1}/m for the physical case of $N = 3$. The danger is that the same might also happen for the rescaling factor between ξ and $\tilde{\xi}$, i.e., that the ratio obtained numerically to first order in $1/N$ may in fact contain the Euler constant which would mask the actual value of the ratio.

In the present communication we address this issue. We compute explicitly the $T-$ independent $1/N$ corrections to both correlation lengths and show that the rescaling factor does not contain the Euler constant. This implies that the $1/N$ result for the ratio is very likely to be trustable, and the rescaling factor between two correlation length is very close to one.

As we already said, in our consideration, we will use heavily results of the $1/N$ expansion for $O(N)$ $\sigma-$model [4,5]. The point of departure for this analysis is the mean-field theory which is exact at $N = \infty$. At the mean-field level, the static structure factor is given by

$$S(k) = \sum_{i=1}^{N} S_{i,i}(k) = \frac{TN_0^2 N}{\rho_s} \frac{1}{m_0^2 + (Q - k)^2} \qquad (5)$$

and $m_0 = (T/c)e^{-2\pi\rho_s/(NT)}$. Consider now finite N. It has been shown in [4,5] that there exist two different types of $1/(N - 2)$ corrections: singular ones which contain $\log(T/m_0)$ and $\log(\log(T/m_0))$, and regular ones, which at small T account for the T-independent renormalizations of $S(k)$ and m. There is a large amount of confidence that logarithmical and double logarithmical perturbation series are geometrical and therefore can be simply exponentiated [8]. Regular $1/(N - 2)$ corrections

require a special care, as we just demonstrated. Collecting both singular and regular $1/N$ corrections and exponentiating the singular ones, one obtains [4]

$$S(k) = 2\pi N_0^2 \frac{N}{N - 2} \left(\frac{(N - 2)T}{2\pi\rho_s}\right)^{\frac{N-1}{N-2}} P(k) \qquad (6)$$

where for k comparable to the inverse correlation length

$$P(k) = \frac{1}{Zm^2 + (Q - k)^2 + \Sigma(k)}. \qquad (7)$$

Here m is given by (2) and Z and $\Sigma(k) \propto (Q - k)^2$ account for a temperature independent $1/(N - 2)$ corrections. For $N = 3$, the functional forms of $S(k)$ and m obtained this way fully agree with the ones obtained in the perturbative RG approach [6].

The expressions for Z and $\Sigma(k)$ have been obtained in [4] but not explicitly presented in that paper. Here we list the catalog of the results which we will need:

$$Z = 1 + \frac{2}{N}\Big(2\log 2 - 1 - $$
$$3\int_0^\infty dx \log\log \frac{x + \sqrt{x^2 + 4}}{2} \frac{x}{(x^2 + 1)^2}\Big);$$
$$\Sigma(k \to Q) = -\frac{4(Q - k)^2}{N} \int_0^\infty dx \log\log \frac{x + \sqrt{x^2 + 4}}{2}$$
$$\times \frac{x(7x^2 - 2)}{(x^2 + 1)^4};$$
$$\Sigma(k = im) = -\frac{m^2}{N} \int_0^\infty dx \log\log \frac{x + \sqrt{x^2 + 4}}{2}$$
$$\times \left(\frac{(x - \sqrt{x^2 + 4})^2}{\sqrt{x^2 + 4}} - 6\frac{x}{(x^2 + 1)^2}\right). \qquad (8)$$

For the two correlation lengths we then obtain

$$\xi^{-2} = m^2 Z(1 + \frac{\Sigma(k = im)}{m^2});$$
$$\tilde{\xi}^{-2} = m^2 Z(1 - \frac{\Sigma(k)}{(Q - k)^2})|_{k \to Q}. \qquad (9)$$

Performing simple manipulations, we find

$$\xi^{-1} = m\left(1 + \frac{1}{N}\left(2\log 2 - 1 - A\right)\right), \qquad (10)$$

where

$$A = \int_0^\infty dx \log\log \frac{x + \sqrt{x^2 + 4}}{2} \left(\frac{(x - \sqrt{x^2 + 4})^2}{2\sqrt{x^2 + 4}}\right). \qquad (11)$$

Introducing $t = \log\frac{x + \sqrt{x^2 + 4}}{2}$ and integrating by parts, we immediately obtain $A = -(\gamma_E + \log 2)$. Substituting this result into (10) we recover Eq. (4). For the ratio of

ξ and $\tilde{\xi}$, the same manipulations yield a more complex expression

$$\tilde{\xi} = \xi \left(1 + \frac{1}{N} \left(\gamma_E + I \right) \right) \qquad (12)$$

where $I = 3I_2 - 14I_3 + 18I_4$, and

$$I_n = \int_0^\infty dt \frac{\sinh t \log t}{(2 \cosh t - 1)^n} \qquad (13)$$

Notice that all integrals I_n are convergent. Physically, this implies that $T-$independent factors in both correlation lengths are determined by system behavior at energy scales which are much smaller than the upper cutoff. At this scales, the behavior is universal and therefore overall factors in ξ and $\tilde{\xi}$ are also universal numbers. Note by passing that similar integrals appear in the calculations of the d.c. Hall conductivity near fractional quantum Hall critical point [9].

To evaluate the integrals (13), we introduce auxiliary function $\Phi_n(t) = \sinh t \log^2(-t)/(2 \cosh t - 1)^n$ and integrate Φ_n over a contour which consists of a circle of an infinite radius and a cut along positive real t. The contour integral yields $-4\pi i I_n$ and simultaneously it is equal to the sum of the residues (modulo $2\pi i$) of the poles along imaginary $t-$axis. Performing calculations and making use of the summation formula

$$\sum_{n=0}^\infty \frac{\log(2\pi n + \pi(1-a))}{2n + (1-a)} - \frac{\log(2\pi n + \pi(1+a))}{2n + (1+a)} =$$
$$\frac{\pi}{2}(\log \pi - \gamma_E) \tan \frac{\pi a}{2} - \int_0^\infty du \frac{\sinh ua}{\sinh u} \log u, \qquad (14)$$

we can explicitly pull out the Euler constant from the integrals

$$I_2 = -\frac{\gamma_E}{2} - \frac{\tilde{I}_2}{2}, \ I_3 = -\frac{\gamma_E}{4} - \frac{\tilde{I}_2}{12} + \frac{\tilde{I}_3}{12},$$
$$I_4 = -\frac{\gamma_E}{6} - \frac{\tilde{I}_2}{18} + \frac{\tilde{I}_3}{36} - \frac{\tilde{I}_4}{36} \qquad (15)$$

where

$$\tilde{I}_2 = \int_0^\infty \frac{\log x}{\sinh \pi x} \frac{\sinh 2\pi x/3}{\sin 2\pi/3},$$
$$\tilde{I}_3 = \int_0^\infty \frac{x \log x}{\sinh \pi x} \frac{\cosh 2\pi x/3}{\cos 2\pi/3},$$
$$\tilde{I}_4 = \int_0^\infty \frac{x^2 \log x}{\sinh \pi x} \frac{\sinh 2\pi x/3}{\sin 2\pi/3} \qquad (16)$$

The analytical expressions for the integrals $\tilde{I}_{3,4}$ have been obtained very recently [10], whereas $\tilde{I}_2$ was known for some time [11]. It turns out that these integrals can be expressed in terms of the derivatives of the Hurvitz Zeta function $d\zeta(x,\alpha)/dx$ at $x = 0, -1, -2$ and $\alpha = 1/6, 1/3, 1/2, 2/3, 5/6, 1$. For $x = 0$, $d\zeta(x,\alpha)/dx =$

$\log(\Gamma(\alpha)/\sqrt{2\pi})$. By analogy, we can introduce generalized Gamma functions via $d\zeta(x,\alpha)/dx|_{x=-n} = \log(\Gamma_{-n}(\alpha)/\sqrt{2\pi})$. Using this definition, we obtain a symbolic representation

$$\tilde{I}_2 = -\log R_0; \ \tilde{I}_3 = 6 \log R_{-1} - 3 \log 6;$$
$$\tilde{I}_4 = 36 \log R_{-2} + 3 \log 6 \qquad (17)$$

where

$$R_{-s} = \frac{\Gamma_{-s}(1/3)\Gamma_{-s}(1/2)}{\Gamma_{-s}(5/6)\Gamma_{-s}(1)} \left(\frac{\Gamma_{-s}(7/6)\Gamma_{-s}(1)}{\Gamma_{-s}(2/3)\Gamma_{-s}(1/2)} \right)^{(-1)^s} \qquad (18)$$

The expression for R_0 and R_{-1} can be reduced to an explicit closed-form expression containing, e.g., logarithms of Gamma-functions, but no Euler constant [12]. No closed-form expression in terms of tabulated functions is known for R_{-2}. It is however quite reasonable to assume that it also does not contain Euler constant.

Assembling now all contributions to I and substituting the result into (12) we find that the Euler constant is cancelled out. The rest is combined into

$$\tilde{\xi} = \xi \left(1 + \frac{1}{2(N-2)} \log[6R_0^{8/3} R_{-1}^{-8} R_{-2}^{-36}] + O\left(\frac{1}{(N-2)^2} \right) \right) \qquad (19)$$

This expression is the central result of the paper.

The next issue is how to account for the higher-order terms in $1/(N-2)$. Here we use the same assumption as was proven to work for ξ, namely that after the Euler constant is subtracted, the rest of the regular $O(1/(N-2))$ correction can be exponentiated. Using this assumption, we finally obtain

$$\tilde{\xi}^2 = \xi^2 \ (6R_0^{8/3} R_{-1}^{-8} R_{-2}^{-36})^{1/(N-2)} \qquad (20)$$

For $N = 3$ this yields $\tilde{\xi}^2/\xi^2 = 0.993$, i.e. the ratio is indeed very close to one. This result may sound intuitively obvious, but is not based on any apparent physical reasons and therefore had to be verified by explicit calculations. This is what we did.

The extreme closeness of the ratio $\tilde{\xi}/\xi$ to 1 is consistent with recent claims that at $T \to 0$, the numerically computed spin correlation length [1,2] approaches the Hasenfratz-Niedermayer result, Eq.(1).

Using our expressions for Z and ξ, we can also compute the overall factor for the structure factor $S(Q)$ which is also studied in numerical simulations. The numerical evaluation of the first $1/(N-2)$ correction yields $P(Q) \equiv 1/(Zm^2) = \xi^2(1 + 0.188/(N-2))$. Exponentiating this result, one obtains $P(Q)/\xi^2 \approx 1.2$. Numerical simulations [2], on the other hand, reported that the actual rescaling factor is more than three times larger than this number. We performed analytical calculations along the same lines as above and obtained

$$P(Q) = \xi^2[1 + \frac{1}{N-2}(2\gamma_E - \log 2 + 6I_2)] \qquad (21)$$

where I_2 is given by (15). Substituting the result for I_2 into this expression, we obtain

$$P(Q) = \xi^2[1 + \frac{1}{N-2}(-\gamma_E + 3\log(R_0) - \log 2)] \quad (22)$$

This result coincides with the one obtained earlier by Campostrini and Rossi [5], and cited previously in [13]. We see now that Euler constant is present in the perturbation series, i.e. one cannot simply exponentiate the lowest-order result. Using the same procedure as before, i.e., treating γ_E as coming from the expansion of $\Gamma(1 + 1/(N-2))$, and exponentiating the rest of (22), we obtain

$$P(Q) = 2^{1/(2-N)}\,\Gamma(\frac{N-1}{N-2})\left(\frac{\Gamma(1/3)\Gamma(7/6)}{\Gamma(5/6)\Gamma(2/3)}\right)^{3/(N-2)}\xi^2$$
$$(23)$$

For $N = 3$, this yields $P(Q)\xi^{-2} = 2.149$ which is about two times larger than the result obtained by formally exponentiating the whole $1/(N-2)$ correction. Still, however, this result does not fully agree with quantum Monte Carlo simulations at low T which reported $P(Q)\xi^{-2} \approx 4$ for both $S = 1/2$ [2] and $S = 1$ [14]. The series expansion results [15] reported somewhat smaller $P(Q)\xi^{-2} \approx 3.2$ for $S = 1/2$. The reason for the discrepancy is not clear to us. Possibly, numerical simulations for $S(Q)$ were performed not deep inside the asymptotic scaling regime at $T \to 0$. Another possibility is that something may be wrong with the exponentiation of the first $1/N$ correction to $S(Q)$, though this is unlikely in view of the results for ξ.

[7] The transformation $N \to N - 2$ is due to the fact that in the renormalized-classical region, the low-temperature behavior of the system is governed by the interaction between would-be Goldstone modes, and a number of them interacting with the given one is $N - 2$.

[8] The confidence is based on the results of the $1/N$ expansion to second order in $1/N$ and on the full agreement, for the physical $N = 3$, between the functional forms of observables, obtained by exponentiation of the leading $1/N$ corrections, and the ones obtained by the perturbative RG treatment [6].

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